Model description PhytoBasinRisk

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General remarks

PhytoBasinRisk is a water quality model to simulate the risk of critical phytoplankton biomass and composition in large river basins. The phytoplankton of rivers is expected to be sensitive to multiple pressures driven by human activity: a) changes in nutrient emissions to and resulting concentration in surface water, b) changes in riparian land cover (i.e. shading, Hutchins et al. 2010; Schöll 1999), and c) climate change effects on discharge, radiation, and water temperature.

Although PhytoBasinRisk operates on arbitrary, independent time steps, the current software can only be used with daily to monthly climate data and monthly nutrient data. The two reasons for the latter restriction are that a) nutrients are typically sampled bi-weekly or monthly and b) their temporal variability is smaller compared to hydro-climatological variables. Growth and loss processes are calculated at one day. Therefore, monthly climate data corresponds to mean daily conditions.

PhytoBasinRisk was originally developed as module and with the output of the model MONERIS (Venohr et al. 2011). Nonetheless, the model can be linked to other water quality or hydrological models. The required topology of sub-catchments (analytical units, sub-basins), henceforth abbreviated as AU, should be taken, together with the model output, from such coupled model.

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Technical specifications and requirements

PhytoBasinRisk is written in Python 2.7 and depends on several mandatory and optional 3rd-party libraries (Table 1). The software itself is platform-independent. However, the Python version (32/64 bit) must match the version of the ODBC driver(s) required for database access. Note that Microsoft Access files can only be opened under Microsoft Windows (read-only).

Table 1. Libraries used by PhytoBasinRisk. Note: The software was developed and used under Windows 32bit.

	Library	**Tested version**	**Purpose**
Mandatory	pandas	0.17.1	Data handling
	numpy	1.10.4	Data handling
	networkx	1.11	Routing
Optional	sqlalchemy	1.0.13	Generic DB access via database drivers in pandas
	psycopg2	2.6.1	Database driver to access Postgres DB
	pypyodbc	1.3.3	… for reading MS Access files (Windows only)
	pyodbc	3.0.10	… for reading MS Access files (Windows only)
	pytables		For caching the results

While table names are user-defined (i.e. program arguments, Table 2), the column and row names must match the values defined at the beginning of the source code (Table 4ff.). The model can be adapted without code changes, e.g. algae groups can be inserted as new rows in the Algae table.

The model results are written as a time-series to the output table. This table can (or must in case of MS Access files) be in a separate database. Caching can be enabled to minimize slow database access. Apart from error messages, the software gives no feedback. The argument *verbose* can be used to increase the verbosity level. In this case, intermediary results are printed to the standard output stream (stdout) which can be redirected to a text file for debugging or other analyses.

Table 2. Content of input database. Table names are arguments. More details in Table 4ff.

Generic table name	**Content**
Subcatchment	AU characteristics (static)
Climate	Time-series: global radiation, length of daytime, Q
Nutrients	Time-series: DIN, TP, SI, T_{water}, TSS, optionally Q (if not in Climate)
Algae	Algae-specific constants
Wrtvelo	Mean velocity (classes) for estimating the water residence time
Constants	Model constants
Output	Time series of cumulated net chlorophyll a (chl-a) and proportion of each algal group, optional in different database
Defined results	Time-series of chl-a as input to downstream AUs (i.e. AUs not simulated)
Default	Default values to replace missing values in the Nutrients table

Pre-processing and model setup

The river basin is spatially divided into AUs which require unique ids. AUs also need to-ids holding the AU id of the downstream neighbor (a second id can be specified to consider water diversion) or some virtual id in case of outlets. In this way, a flow network (topology) directed downstream is created which must not contain any cycle (i.e. a directed acyclic graph). Such a “flow equation” should be taken from nutrient or hydrological models if their output is used as model input.

The riparian vegetation has to be derived from land-use maps. The shading factor (shad_fac) is calculated from the relative area covered by trees and bushes in the 10m-buffer zone (ctb), assuming more shading by trees (up to 80%) than by bushes (up to 60%). Shading also depends on river width, ranging from 100% (5-6 m width, DeWalle 2010) to 0% (≥30 m) (Eq. 1).

Eq. 1: $\text{shad\_fac} = \text{ctb} \cdot 1.5749\, e^{-0.092 \cdot \text{width}}$

Slope and altitude are derived from digital elevation models. Global radiation and water temperature are interpolated from monitoring stations or estimated from ancillary data like air temperature if not readily available as gridded data. The total runoff is normally provided by hydrological models. The mean water discharge (MQ) is calculated as the long-term (LT) average discharge of the time series if not separately provided (e.g. for scenario calculations).

Further stream and flow characteristics like river length, width, water depth under MQ conditions, number of deep lakes (derived from WFD types “stratified lakes”), and the percentage of lake area to total water surface area are also needed (cf. Table 4ff.) and land-use and other geodata (e.g. the official ATKIS geodata in Germany). As PhytoBasinRisk considers main rivers (MR which connect AUs) and tributaries (TRIB, within AUs), input values must be derived separately for both categories (see table 4 and 5).

Model flow

After some basic checks, the software loads all input data from the input database into pandas data-frames for further processing. After establishing the flow network from the ids in the subcatchment table, ids with known output (Defined results) are removed from this network. The sub-catchments are topologically sorted from headwaters to outlets and processed. This ensures that the results of upstream areas are available. For each area, the whole time-series including the output of upstream neighbors is read, merged, and processed (after optionally filling gaps with the Default table).

In addition to the following description of model flow, the Excel-file named "doku_para_M_PhytoBasinRisk_webpage.xlsx" is an example framework to illustrate the calculation steps for chlorophyll a for one subcatchment (1 spatial analytic unit).

Algae-specific growth and loss are calculated for each AU and routed downstream along the river network (Eq. 2). At confluences, the output of upstream areas is weighted by discharge. Both, growth and loss happen during the calculated water residence time but not longer than 1 day, which is the basic time step for river segments. Lakes are handled with specific assumptions. The output concentration of chl-a of any algal group is set to a (user-defined) minimum value (inoculum).

Eq. 2: chla_out = max(chla_growth + chla_in - chla_loss, inoculum)

Water residence time

The water residence time (WRT) in AUs is the sum of the WRT of rivers (WRT_{riv}) and of lakes (WRT_{lake}). WRT_{riv} is estimated from the total river length (rl), flow velocity (v) under long-term mean conditions and current flow, with specific exponents k for main rivers and tributaries (Eq. 3).

Eq. 3: $WRT_{riv} = rl \cdot v \cdot e^{((Q / Q\_LT) \cdot k)}$

WRT_{lake} might be unavailable. For the Middle Elbe basin, for instance, we assumed that each km lake length increases the WRT by factor 1.1 and each deep lake by 30 days. The maximal WRT for algal growth is 1 day.

For each AU, WRT class values are assigned to MR and TRIB which are translated to flow velocity (Table 3, table Wrtvelo). For the Elbe Basin, the observed flow velocity of smaller rivers (BLfW 2002) as well as of the Elbe and some of its tributaries (IKSE 2005; Köhler et al 2002) were used to define theses classes. They were then applied to all AU taking slope and river width into account.

Table 3. Average values of flow velocities (m/s) under mean flow condition in the Elbe basin

WRT class MR	**v (m/s)**	**WRT class TRIB**	**v (m/s)**
10	0.2	1	0.03
14	0.35	2	0.08
9	0.5	3	0.3
12	0.75	4	0.8
8	1	5	1.2
11	1.2	6	1.4
		7	2.5

The velocity classes are obtained from MQ conditions and are modified according to the ratio of current Q and MQ. An exponent describes how strong the velocity changes with Q. The exponent can be derived from observed velocity-discharge relationships for mean, high, and low flow conditions. PhytoBasinRisk uses different exponents for MR and TRIB (Table 9).

Growth and limitation functions

Following the strategy of Reynolds & Irish (1997) for the model ProTech (Elliot et al. 2000, 2006), algae-specific growth rates under ideal culture conditions during the WRT are assumed. However, maximum growth (chla_opt) can be limited by light (L), nutrients (N), and water temperature (T). To calculate the effective growth, these limitations are applied as relative correction factors f as it is realized in model Q-Sim (Kirchesch & Schöl 1999; Quiel et al. 2011; Eq. 4).

Eq. 4: $\text{chla\_net} = \text{chla\_opt} \cdot fT \cdot fN \cdot fL$

Light availability

Riparian shading, reflection at the water surface, and absorption in the water column (depending on dissolved substances, colour, and depth) reduce the incoming global radiation. PhytoBasinRisk follows the QSim approach of Hardenbicker et al. (2014) which assumes fully mixed water bodies (1D model). In addition, PhytoBasinRisk dynamically estimates river depths (no gauges needed). The changing water level is included because water depth is a crucial input parameter not only for light availability for algae growth (Köhler et al. 2002) but also for losses (e.g. mussels). We also consider riparian shading as an important factor for rivers smaller than 30 m width with an externally derived shading factor based on landuse in riparian zones.

The water depth at gauge stations might not be available in sufficient spatial resolution. Furthermore, artificial river bed cross-sections at gauges can hamper the extrapolation to other stretches. For the Middle Elbe basin, for example, we estimated the water depths under mean flow (MQ) in all AUs by extrapolating a depth-width-relationship available for selected main rivers and tributaries (IKSE, 2005). The exponent (HQf in Table 4) describes the river-specific relationship between discharge and depth as derived from observed flow-depth curves. Using this exponent and the ratio of actual discharge to MQ, the water depth is estimated for each time step. PhytoBasinRisk also supports AU-specific values to cope with heavily modified water bodies like river Spree in Berlin.

Nutrients

Nutrient limitation is defined by the most limiting nutrient (Liebig's law). For each algal group, the half-saturation constant k of P, N, and Si is compared to the incoming nutrients (conc_in) and converted to the limiting factor f (Eq. 5, Quiel et al. 2011).

Eq. 5: $fN = \min(\text{conc\_in}[N, P, Si] / (k[N, P, Si] + \text{conc\_in}[N, P, Si])$

Water temperature

Similar to nutrients, we use a temperature which enables half-optimal growth (kT) to quantify the limiting effect of temperature below the optimal temperature for growth (T_{opt}).

Eq. 6: $fT = T_{water} / (kT + T_{water})$ if $T_{water} < T_{opt}$, or 1 otherwise

Losses

For each time step, the losses are calculated according to Eq. 7. Similar to growth, sedimentation, grazing, and mortality also happen during the water residence time which is limited to 1 day.

Eq. 7: chla_out = chla_net - chla_sed - chla_graz - chla_mort

Sedimentation

In some sub-catchments lakes have a high share of the total water surface areas resulting in high sedimentation losses of the potamoplankton. So, a fixed loss value near maximum sedimentation is applied in PhytoBasinRisk when lakes cover more than 50% of the surface water. Where lakes are less relevant, the sedimentation loss depends on lake length (ll in km) and the WRT (Eq. 8). The factor f_sed is the sedimentation factor in km^{-1} d^{-1}. The negative exponent k (LENGTH_EXPONENT in Table 9) ensures that the sedimentation rapidly increases within the first kilometer but less so afterwards, a spatial dynamic of large particles which can be observed after flood events into reservoirs.

Eq. 8: $chla\_sed = ll^{(1+k)} \cdot f\_sed \cdot WRT$

Grazing

Grazing loss by zooplankton (ciliats, rotifers) is set to 10% if cumulated WRT is longer than 3 days to simulate grazing in stagnant water. In flowing waters, rotifers can also be important (Holst 2006). The abundance of rotifers is estimated from chlorophyll a and water temperature for broad river stretches (for the Middle Elbe we used 35 m as threshold). Grazing is calculated from individual ingesting rates of 2.9 µg C/d (Quiel et al. 2011) which corresponds to 0.0138 µg/L chl-a.

Grazing loss by mussels and macrozoobenthos is calculated from river depth, assuming that mussel grazing is highest in shallow river beds with long residence time (Lindim 2015).

Mortality

Mortality is low for algae and is set to 0.1% (Quiel et al. 2011, Hutchins et al. 2010).

Outlook

PhytoBasinRisk was primarily developed for the Middle Elbe basin in Germany (Mischke et al. 2016). Prior any application elsewhere, the model assumptions and constants must be analyzed in more detail with simulated and empirical data. For instance, discharge-flow time curves from monitoring gauges can be used to refine the WRT estimation. The model can easily adapted to river-specific processes by changing the values in the constant table and by detailed sub-catchment data. Without code changes the model can consider, e.g., functional algal traits or species instead of the four algal classes.

Other adaptations will require code changes, like

- Using daily instead of monthly nutrient data
- Considering WRT as a delay if WRT > 1 day

- Including other database drivers: the pandas library uses SQLAlchemy engines/connections for querying DB, SQLAlchemy supports internal and external dialects other than PostgreSQL to communicate with DBs (http://docs.sqlalchemy.org/en/latest/dialects/index.html)

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Table 4. Required columns in Sub-catchment table ("au_characters") and variable names in source code, for main rivers (mr) and tributaries (trib)

Variable name	**Column name for value**	**Unit**	**Comment**
AREA_ID	from_id	-	AU id
TO_ID	to_ID	-	AU id downstream
WIDTH_TRIB	widthtrib_riv	m	Mean river width
WIDTH_MR	widthmr_riv	m	
H_TRIB	h_trib	m	Water depth under MQ conditions
H_MR	h_mr	m	
LENGTH_TRIB	lengtrib_riv	m	River length without lakes
LENGTH_MR	lengmr_riv	m	
LENGTH_LAKE_MR	mr_length_lake	m	Lake length
LENGTH_LAKE_TRIB	trib_length_lake	m	
N_DEEPLAKE_MR	mr_n_deep_lake	-	Number deep lakes
N_DEEPLAKE	trib_n_deep_lake	-	
LAKE_PROP_AREA_TRIB	laketrib_prop_area	%	Lake to total water area
LAKE_PROP_AREA_MR	lakemr_prop_area	%	
SLOPE	slope	%	For WRTvelo table (unused)
BOGVAR	bogvar	-	Correction factor light availability humic substances
SHAD_TRIB	trib_shad_fac	-	Shading factor
SHAD_MR	mr_shad_fac	-	
WRT_class_MR	wrt_class_mr	-	Unique id, defined in WRTvelo
WRT_class_TRIB	wrt_class_trib	-	
HQ_EXPONENT_TRIB	hqf_trib	-	Exponent for rating curve (depth-discharge relationship)
HQ_EXPONENT_MR	hqf_mr	-	

Table 5. Required columns in Climate and Nutrient tables and variable names in source code

Variable name	**Value**	**Unit**	**Comment**
AREA_ID	from_id	-	Identical to Table 4
DATE	datum	-	Date (YYYY-MM-DD)
Q	q	m^3/s	Discharge, preferably in Climate table (discharge of sub-catchment)
GRAD	gr	J/cm2/day	Global radiation
TLIGHT	tlight	hours	Day light
SI_ON	si_on	mg/L	Si concentration
N_ON	n_on	mg/L	DIN concentration
P_ON	p_on	mg/L	TP concentration
TSS	ss	mg/L	Total suspended solids, dry weight
WTEMP	temp_in	°C	Water temperature

Table 6. Optional columns in Subcatchment table and variable names in source code, for main rivers (mr) and tributaries (trib)

Variable name	Value	Unit	Comment
TO_ID2	to_id2	-	Secondary to_id
TO_SPLIT	splitting	-	Share of Q to primary to_id
LT_Q_TRIB	lt_q_trib	m^3/s	MQ (long-term mean Q)
LT_CUMQ	lt_q_mr	m^3/s	If missing calculated from time-series

Table 7. Required columns in Algae table and variable names in source code

Variable name	Value	Unit	Comment
ALGAL_GRP	algal_group	-	Unique identifier
kSI	ksi	-	Half-saturation constant for Si
kN	kn	m^3/s	Half-saturation constant for N
kP	kp	$J/cm^2/day$	Half-saturation constant for P
MY	my	1/day	Growth rate per day
kT	kt	°C	Assumed temperature which enables half of the optimal growth
TEMP_OPT	t_opt	°C	Optimal temperature for growth
ACSTART	acstart_perc	%	Share of initial chl-a in tributaries (see START_CHLA in Table 9)
LF1	lf_1	-	Empirical coefficient light limitation function $y = LF1 \cdot I_0^2 + LF2 \cdot I_0 - LKsub$
LF2	lf_2	-	Empirical coefficient light limitation function $y = LF1 \cdot I_0^2 + LF2 \cdot I_0 - LKsub$
LKsub	lk_sub	-	Empirical coefficient light limitation function $y = LF1 \cdot I_0^2 + LF2 \cdot I_0 - LKsub$

Table 8. Optional columns in Algae table and variable names in source code, relative weighting factors, sum of all algae groups must be 1.0 if specified, algae groups are equally weighted if missing.

Variable name	Value	Unit	Comment
WGH_SEDIM	factor_sed	-	Weighting factor sedimentation loss
WGH_GRAZ	factor_graz	-	…grazing (zooplankton)
WGH_MUS	factor_mus	-	…grazing (mussels)

Table 9. Required row names in Constants table and variable names in source code, for main rivers (mr) and tributaries (trib)

Usage	Variable name	Value	Unit	Comment
Light	CHLA_AB	ABSCHLA	1/m	Absorption coefficient chl-a
	HS_ABS	ABSHS	1/m	Absorption coeff. humic substances
	TSS_ABS	ABSSS	1/m	Absorption coeff. suspended solids
	HS_CONST	HS_CONSTANT	mg/L	Correction of BOGVAR (Table 4)
	CF	CF	-	Global radiation to PAR (µE m^2/s)
	RF	RF	-	Reflection factor
	START_SHADOW	START_SHADOW	month	Start shading of riparian vegetation

	END_SHADOW	END_SHADOW	month	End shading of riparian vegetation
WRT	F_WRT_LAKE	F_WRT_LAKE_KM	1/km	Rel increase of WRT with lake length
	WRT_DEEPLAKE	WRT_DEEPLAKE	day	Increase of WRT for each deep lake
	WRT_EXP_TRIB	QDIF_EXP_TRIB	-	Exponent TRIB, $(q\_trib/lt\_q\_trib)^{exp}$
	WRT_EXP_MR	QDIF_EXP_MR	-	…for MR
Growth	START_CHLA	TRIB_CHLA_IN	µg/L	Initial chl-a in tributaries
	MIN_TRIB_LENGTH_STARTCHLA	MIN_TRIB_LENGTH_STARTCHLA	km	minimum length of tributaries to apply correction to START_CHLA
	TRIB_LAKE_PROP_STARTCHLA	TRIB_LAKE_PROP_STARTCHLA	µg/L	to consider lakes - value added to START_CHLA
	MIN_MR_LENGTH_INCHLA	MIN_MR_LENGTH_INCHLA	km	same for MR to correct input chl-a from upstream areas
	MR_LAKE_PROP_INCHLA	MR_LAKE_PROP_INCHLA	µg/L	to consider lakes - value added to START_CHLA
Loss	LENGTH_EXPONENT	LENGTH_EXPONENT	-	Exponent for lake length, for sedimentation
	THRESH_PROP_LAKE_AREA	TH_PROP_LAKE_AREA	%	Sedimentation loss, threshold proportion lake area
	MAX_SED_LOSS	MAX_SED_LOSS	-	Maximum sedimentation loss
	F_SED_KM_D	F_SED_KM_D	$km^{-1}\ d^{-1}$	Sedimentation factor lake length
	THRESH_GRAZ_DAYS	TH_GRAZ_DAYS	d	Grazing zooplankton, threshold WRT
	F_GRAZ_ZOO	F_GRAZ_ZOO	1/d	Relative loss due to maximal grazing zooplankton
	THRESH_RIV_DEPTH	TH_RIV_DEPTH	m	Grazing mussels, threshold depth
	F_GRAZ_MUS	F_GRAZ_MUS	-	Relative maximal loss grazing mussels in shallow rivers
	CHLA_MORT	F_CHL_MORT	-	Mortality loss, fixed for all algae
	TH_WIDTH_MR_ROTI	TH_WIDTH_MR_ROTI	m	Threshold “broad” river segments for estimation abundance rotifers
	MIN_TEMP_ROTI	MIN_TEMP_ROTI	°C	Threshold water temperature for estimating number of rotifers
	REGR_FACTOR_CHLA_ROTI	REGR_FACTOR_CHLA_ROTI	-	Coeff. a rotifer model, $y = a \cdot e^{bx}$
	REGR_EXP_CHLA_ROTI	REGR_EXP_CHLA_ROTI	-	Coeff. b rotifer model, $y = a \cdot e^{bx}$
	MAX_CHLA_ROTI	REGR_MAX_CHLA_ROTI	µg/L	Max. chl-a value in rotifer model
	DAILYC_INGEST_ROTI	DAILYC_INGEST_ROTI	g/ind	Daily C ingestion of rotifers
	REGR_FACTOR_BIOVOL_CHLA	REGR_FACTOR_BIOVOL_CHLA	-	Coeff. a model chl-a loss $y = a X + b$
	REGR_OFFSET_BIOVOL_CHLA	REGR_OFFSET_BIOVOL_CHLA	-	Coeff. b model chl-a loss $y = a X + b$
Output	INOCULUM	INOCCULUM	µg/L	Min. chl-a concentration for algae
Other	HQ_MINQ_MR_TRIB	HQ_MINQ_MR	m3/s	Threshold MQ: exponent of rating curve (HQ_EXPONENT_* in Table 4)
	MIN_Q	MIN_Q	m3/s	Min Q value no flow / negative days

Table 10. Required column names in Wrtvelo table and variable names in source code, for main rivers (mr) and tributaries (trib)

Variable name	Value	Unit	Comment
WRT_VELO_MR	wrt_class_mr	-	WRT_class_MR (Table 4)
WRT_VELO_TRIB	wrt_class_trib	-	WRT_class_TRIB (Table 4)
VELO_VALUE	velo_const	m/s	Flow velocity for WRT class

Table 11. Required column names in Default table and variables in source code. Parameter names must match the values of SI_ON, P_ON, and N_ON in Table 5

Variable name	Value	Unit	Comment
DEF_COLNAME	parameter	-	Column name in Nutrients table
DEF_VALUE	value	mg/L	Default value

Table 12. Columns in Defined table and variables in source code. Values are copied to Output table, mr for main rivers

Variable name	Value	Unit	Comment
AREA_ID	from_id		Identical to Table 4
DATE	datum		Identical to Table 5
Q	q	m^3/s	Cumulated discharge
OUT_CHLA	total_out_chla	µg/L	Total output Chl-a
WIDTH_MR	widthmr_riv	m	Identical to Table 4 or max upstream
COL_ALG_SH_CHLA	chla_+ALGAL_GRP	%	Share of algae groups in Table 7

Table 13. Columns in Output table and variable names in source code. Use argument *–full* for intermediary results, for main rivers (mr) and tributaries (trib)

Variable name	Value	Unit	Comment
AREA_ID	from_id		Identical to Table 4
DATE	datum		Identical to Table 5
Q	q	m^3/s	Cumulated discharge
OUT_CHLA	total_out_chla	µg/L	Total output chl-a
WIDTH_MR	widthmr_riv	m	Identical to Table 4 or max upstream
WEIGHTQ_MR	mr_weightq	-	Share of upstream Q on total Q
WEIGHTQ_TRIB	trib_weightq	-	Remainder (Q TRIB)
WRT_MR	wrt_mr	d	Local WRT (MR)
WRT_TRIB	wrt_trib	d	…TRIB
WRT_UPSTR	mean_in_wrt	d	Discharge-weighted average water residence time of upstream areas
H_MR_MOD	h_mr_mod	m	Estimated current water depth (MR)
H_TRIB_MOD	h_trib_mod	m	…TRIB